

A Domain Decomposition Method for Pseudo-Spectral Electromagnetic Simulations of Plasmas

Jean-Luc Vay, Lawrence Berkeley Nat. Lab.

Irving Haber & Brendan Godfrey, U. Maryland

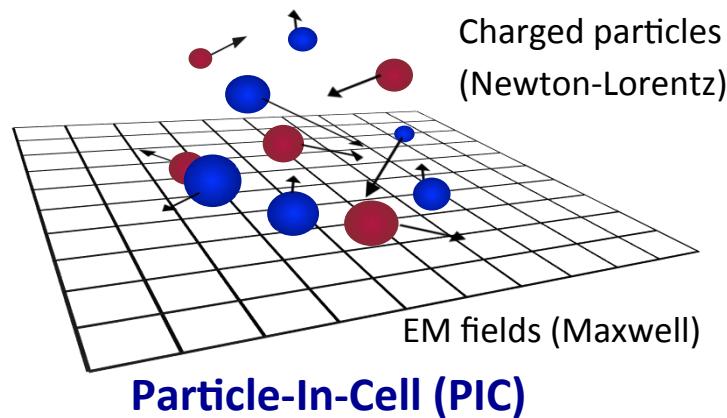
PPPS 2013, San Francisco, CA, U.S.A.



**SciDAC-III
ComPASS**



Particle-In-Cell method is ubiquitous for kinetic modeling of space and laboratory plasmas



PIC is the method of choice for simulations of plasmas and beams

- first principles → includes nonlinear, 3D, kinetic effects,
- scales well to >100k CPUs and burns tens of millions of hours on U.S. supercomputers.

Usual FDTD field solver scales well but impose serious limits on

- time step, accuracy, stability, etc.

Spectral solvers do not scale well but offer

- higher accuracy and stability,
- eventually no time step limit (i.e. no Courant condition on field push).



Analytic spectral solver for Maxwell's equations



In the early 70s, it was shown by Haber et al¹ that an exact solution exists for Maxwell in Fourier space if source \mathbf{J} assumed constant over time step:

"Pseudo-Spectral Analytical Time-Domain" or PSATD

$$\tilde{\mathbf{E}}_L^{n+1} = \tilde{\mathbf{E}}_L^n - \Delta t \tilde{\mathbf{J}}_L^{n+1/2}$$

$$\tilde{\mathbf{E}}_T^{n+1} = C \tilde{\mathbf{E}}_T^n + i S \hat{\mathbf{k}} \times \tilde{\mathbf{B}}^n - \frac{S}{kC} \tilde{\mathbf{J}}_T^{n+1/2},$$

$$\tilde{\mathbf{B}}^{n+1} = C \tilde{\mathbf{B}}^n - i S \hat{\mathbf{k}} \times \tilde{\mathbf{E}}^n + i \frac{1-C}{kC} \hat{\mathbf{k}} \times \tilde{\mathbf{J}}^{n+1/2},$$

with $C = \cos(kc\Delta t)$ and $S = \sin(kc\Delta t)$.

- Note: taking first terms of Taylor expansion of C and S leads to pseudo-spectral formulation:

"Pseudo-Spectral Time-Domain" or PSTD²

$$\tilde{\mathbf{E}}^{n+1} = \tilde{\mathbf{E}}^n + ic\Delta t \mathbf{k} \times \tilde{\mathbf{B}}^{n+1/2} - \Delta t \tilde{\mathbf{J}}^{n+1/2},$$

$$\tilde{\mathbf{B}}^{n+3/2} = \tilde{\mathbf{B}}^{n+1/2} - ic\Delta t \mathbf{k} \times \tilde{\mathbf{E}}^{n+1}.$$

¹I. Haber, R. Lee, H. Klein & J. Boris, *Proc. Sixth Conf. on Num. Sim. Plasma*, Berkeley, CA, 46-48 (1973)

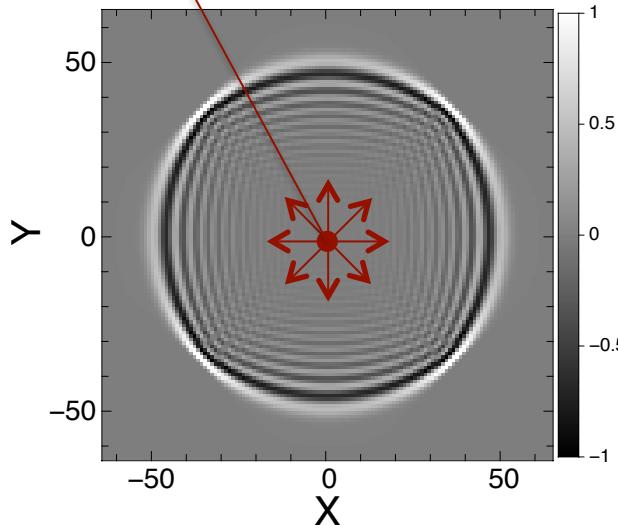
²Similar to UPIC solver, V. Decyck, UCLA

Spectral advantage on expansion of unit pulse

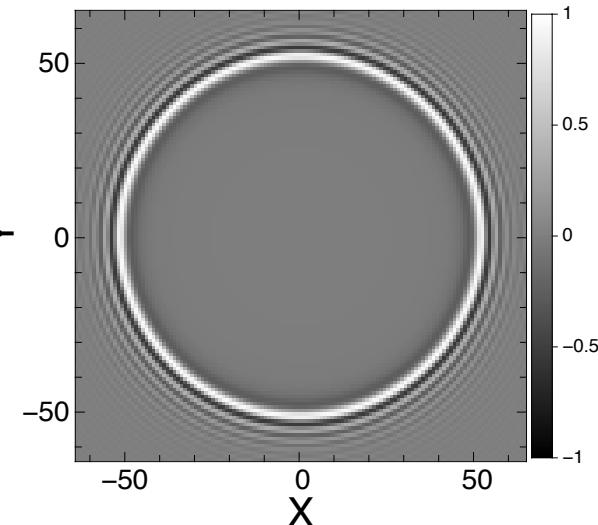
Kronecker

δ pulse

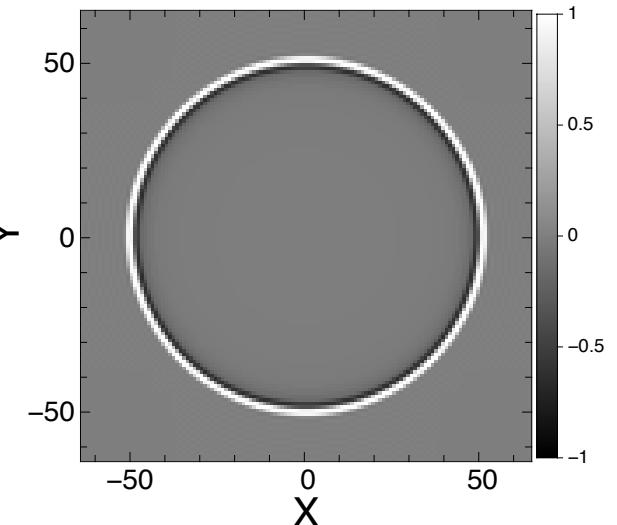
FDTD



PSTD



PSATD



- Numerical dispersion,
- anisotropy,
- Courant condition:

$$c\Delta t \leq 1/\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$$

- Numerical dispersion,
- isotropy,
- Courant condition:

$$c\Delta t \leq 2/\pi \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$$

- Exact dispersion,
- isotropy,
- Courant condition:

None

But spectral method involves global operations:

→ hard to scale to many cores.

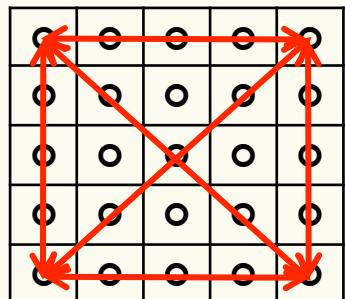
Finite speed of light ensures that

- changes propagate a finite distance during a time advance

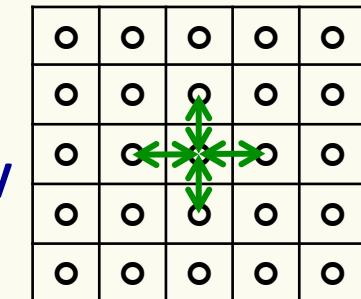
enabling the use of local Fourier Tr.

Replacing

global “costly”



local “cheap”



by

communications

Hard to scale

Easy to scale

*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

New concept* enables scaling of spectral solvers -- using property of Maxwell's equations

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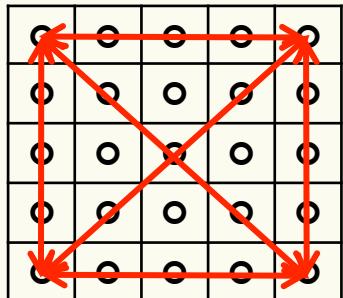
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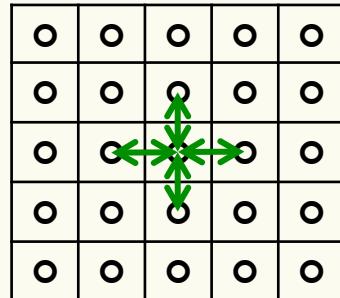
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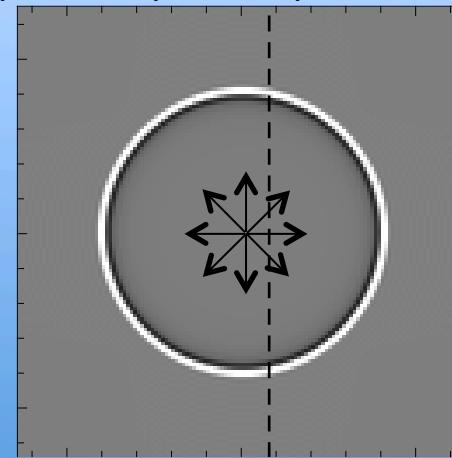


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Example: unit pulse expansion at time T



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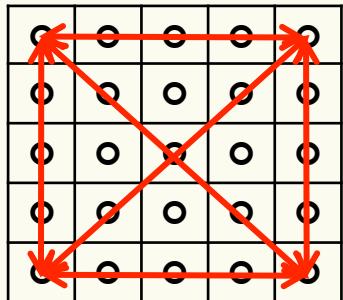
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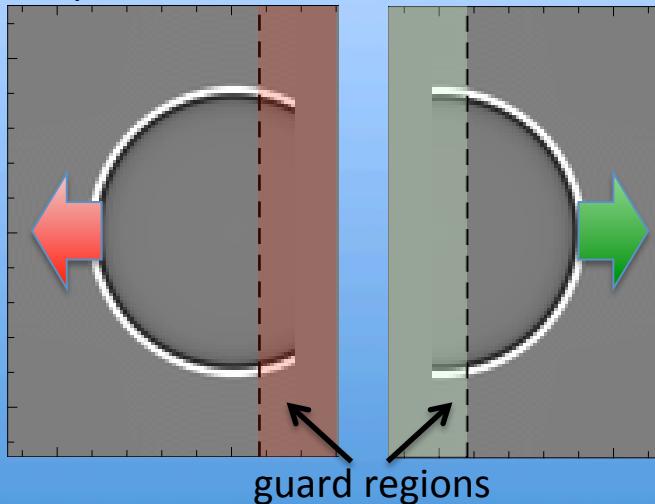


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Separate calculation in two domains



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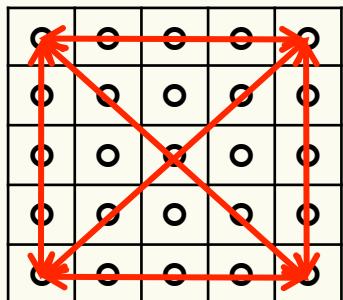
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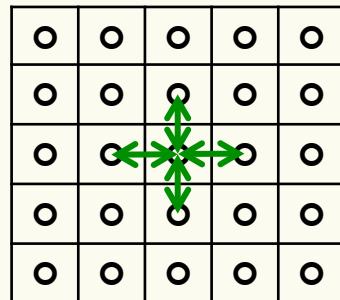
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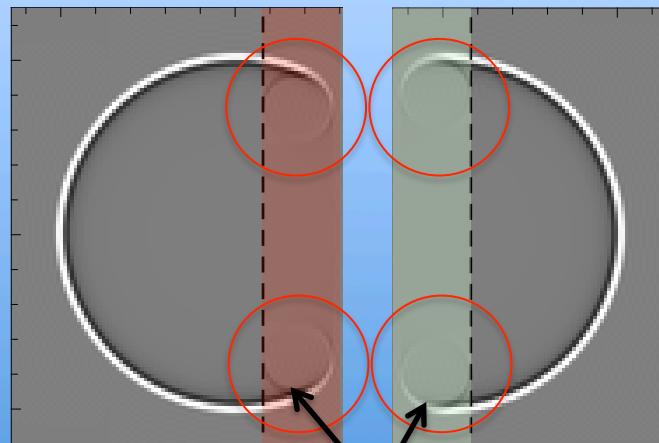


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Advance to time $T + \Delta T$



spurious signal limited to guard regions

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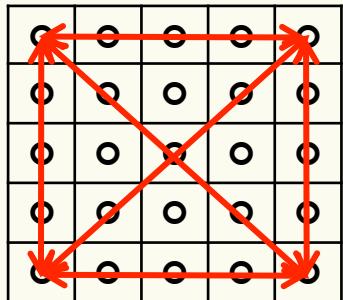
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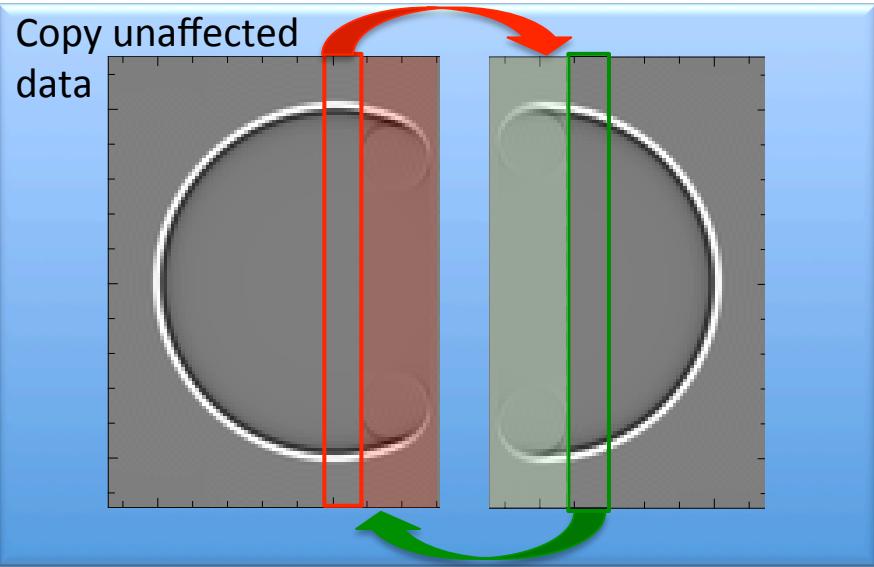
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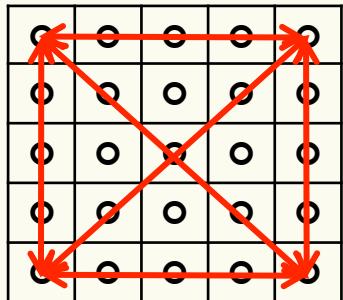
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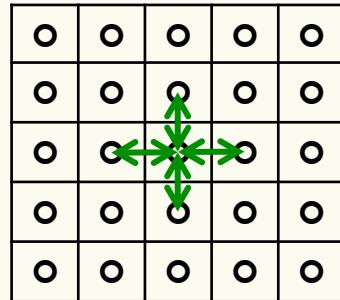
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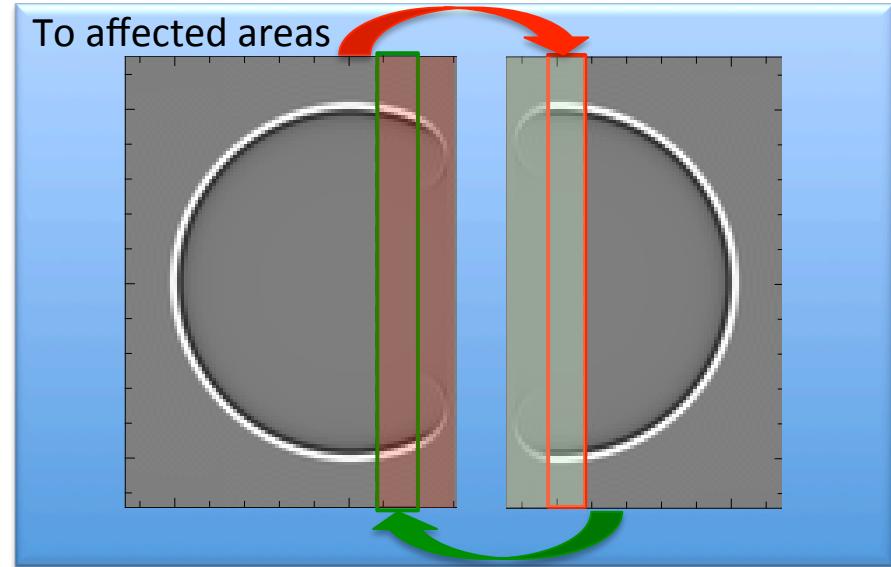
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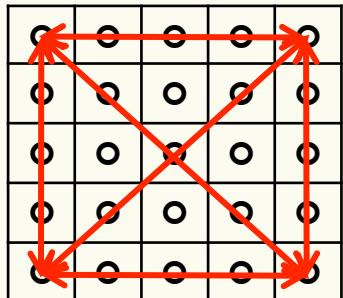
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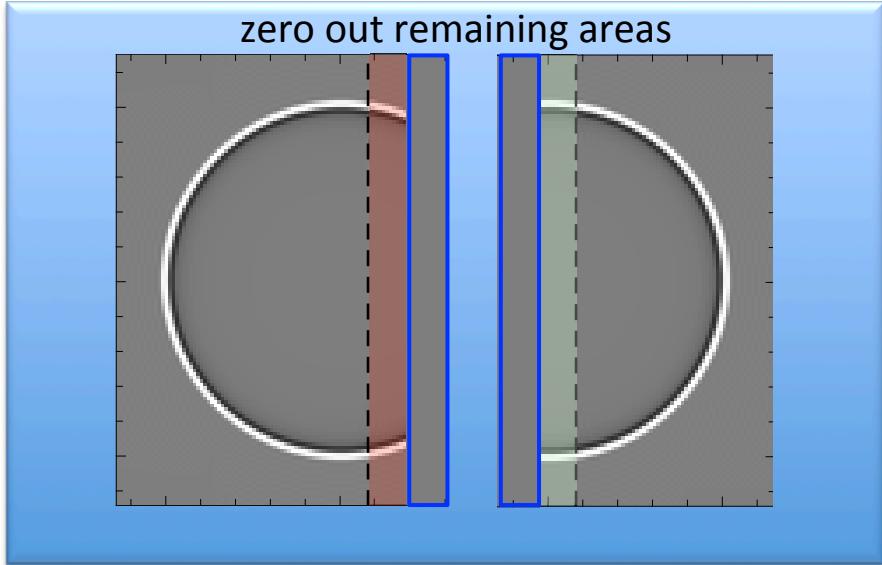
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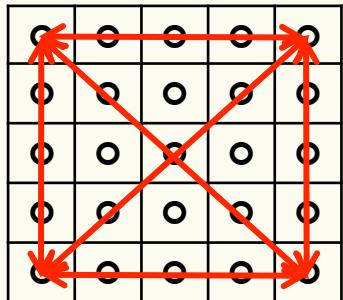
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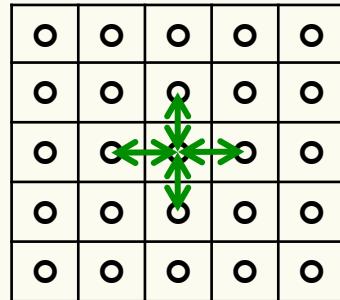
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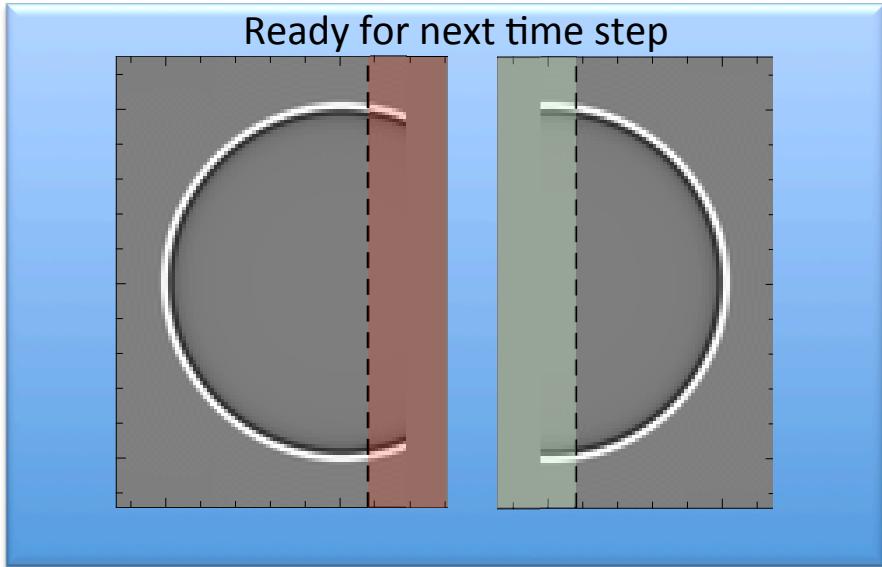
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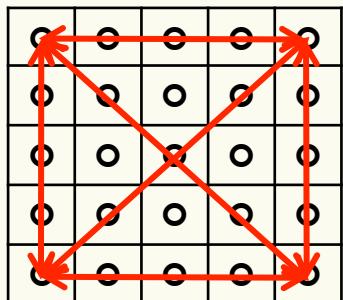
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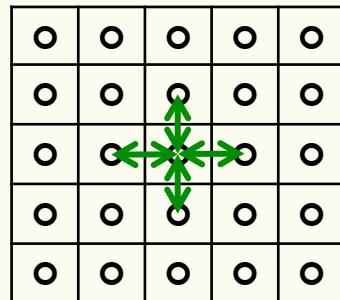
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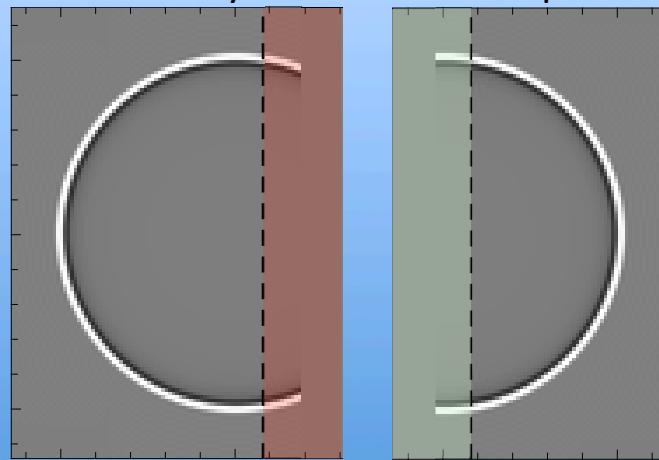
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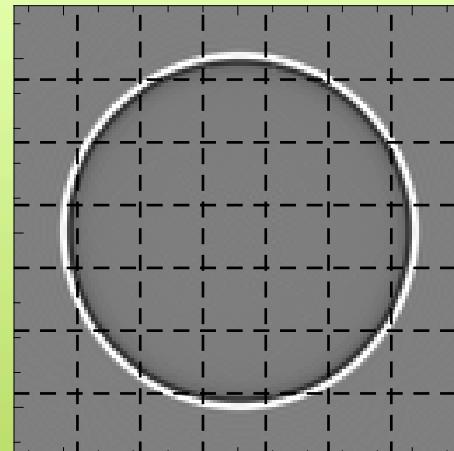


Easy to scale

Ready for next time step



Successfully tested on 7x7 domain



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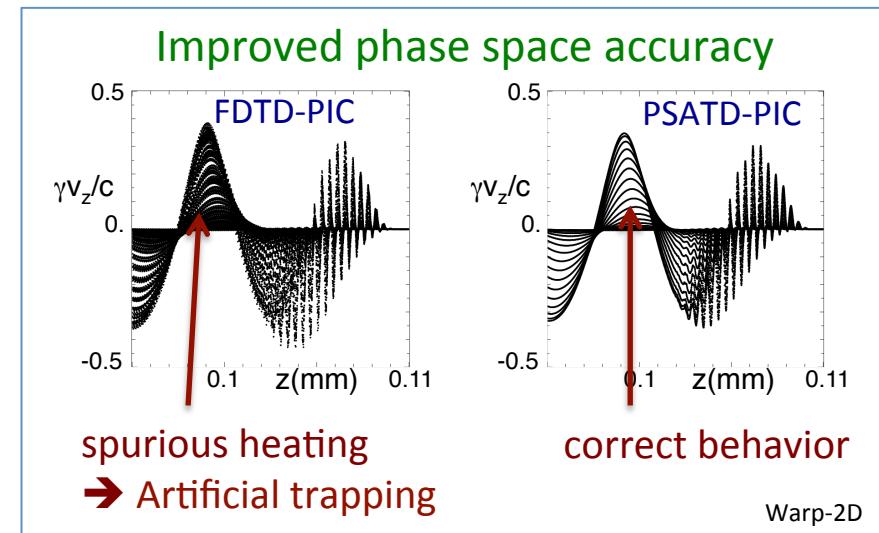
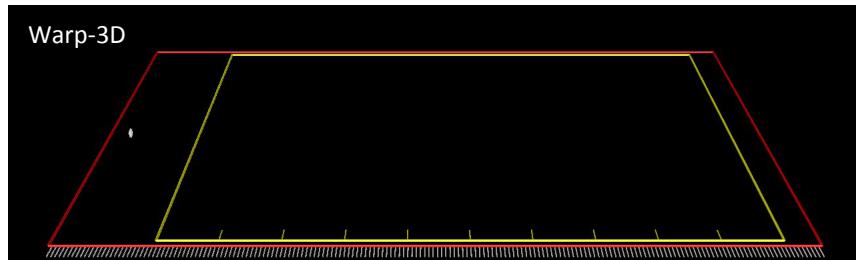


New scheme successfully applied to modeling of laser plasma accelerators with Warp¹



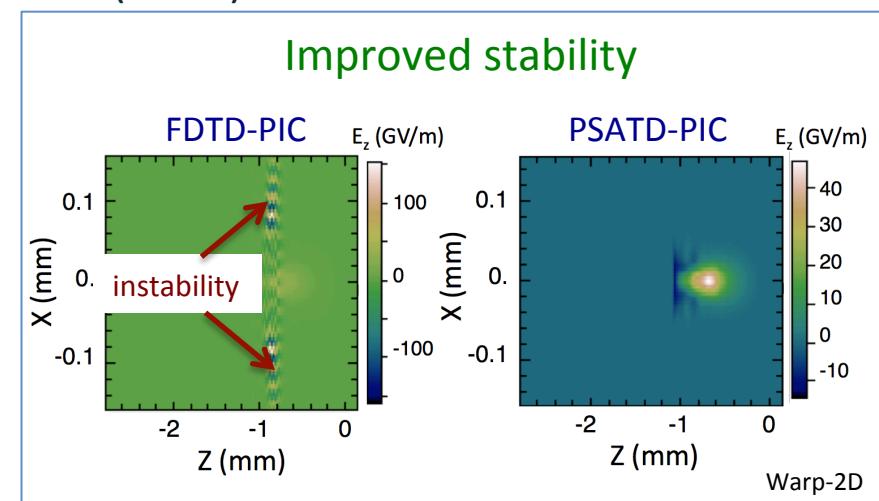
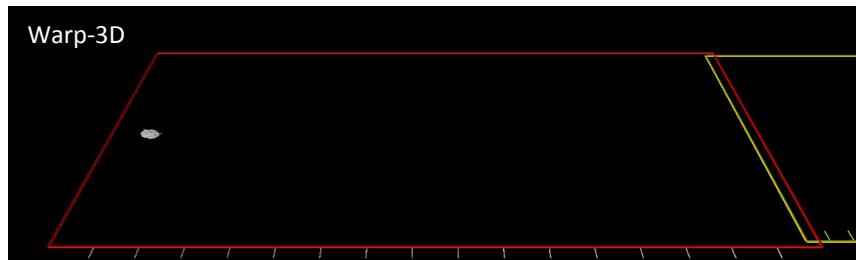
Lab frame

Short laser propagates into long plasma channel,
electron beam accelerated in wake.



Lorentz boosted frame (wake)

Modeling in a boosted frame reduces # time steps².
Plasma drifting near C may lead to Num. Cherenkov.

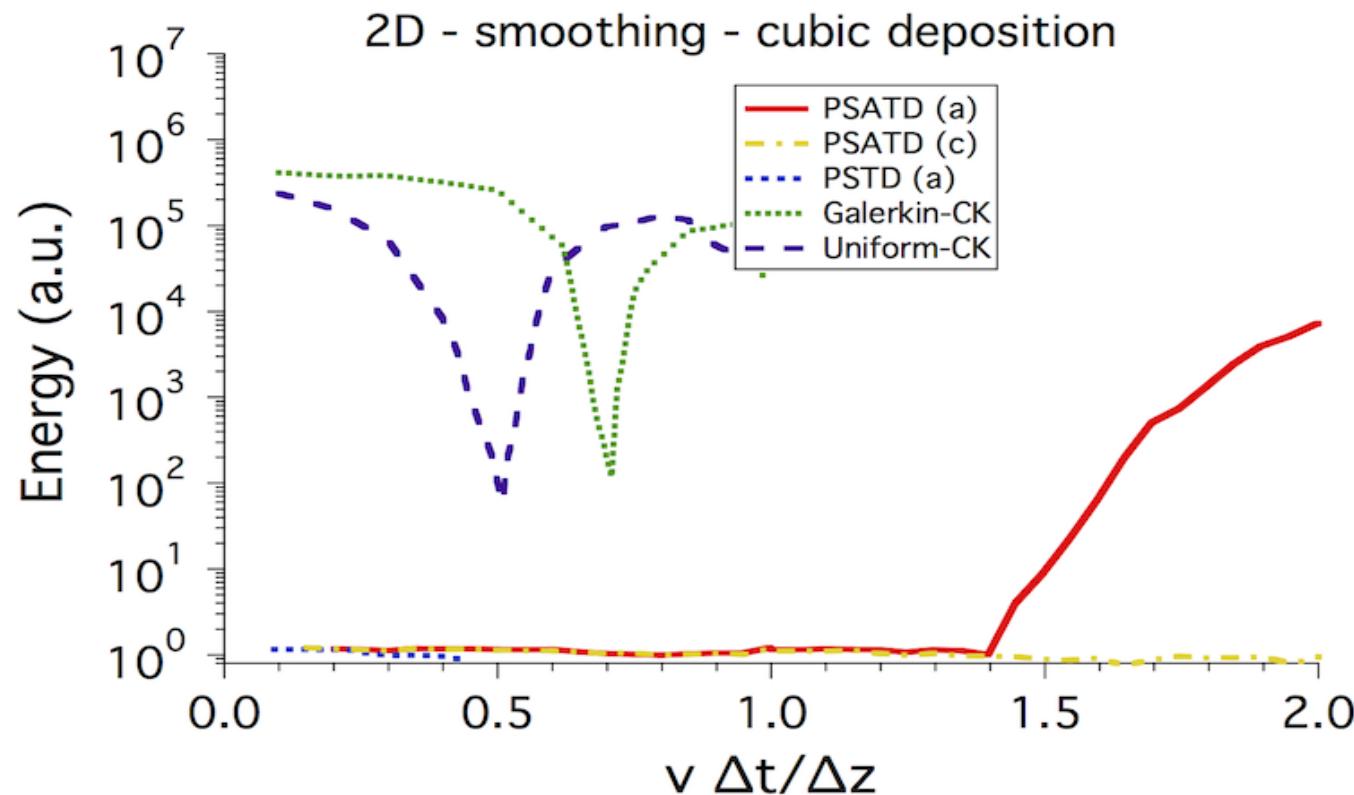


¹A. Friedman, et al., PPPS 2013, paper 4A-3, Tuesday 6/18/2013, 17:00 Grand Ballroom B “Birdsall Memorial Session”

²J.-L. Vay *Phys. Rev. Lett.* **98**, 130405 (2007); ³B. B. Godfrey *J. Comput. Phys.* **15** (1974)



Theory extended to 3-D by Godfrey confirms improved stability*

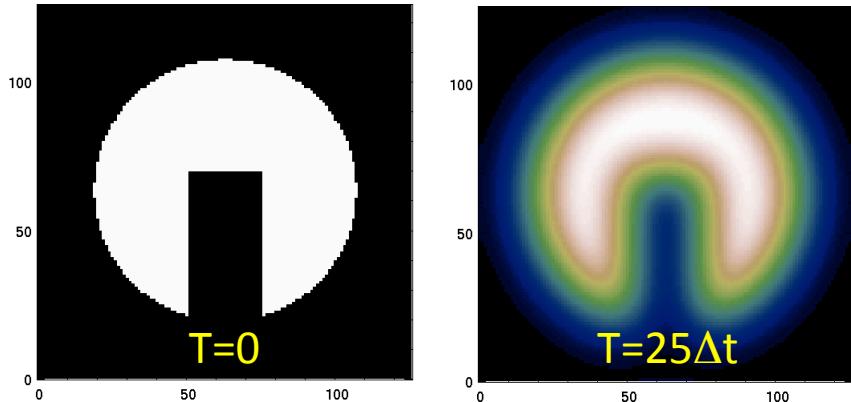


- Numerical energy growth in 3 cm, $\gamma=13$ LPA segment
- FDTD-CK simulation results included for comparison

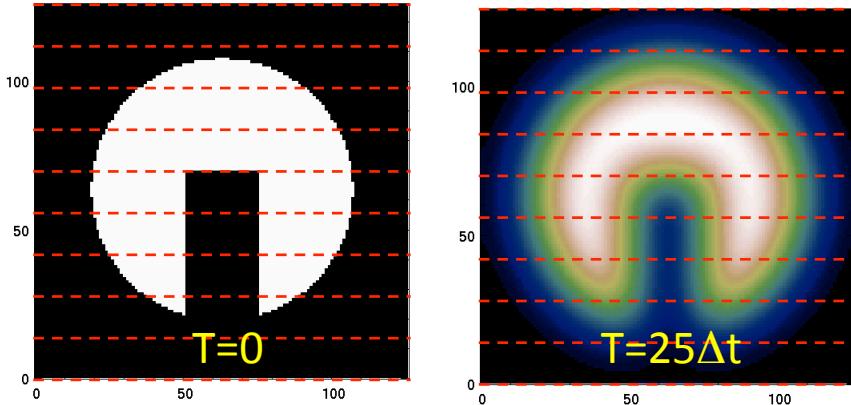
*B. B. Godfrey, et al., PPPS 2013, paper 4A-6, Tuesday 6/18/2013, 17:00 Grand Ballroom B “Birdsall Memorial Session”

- Electromagnetic MHD/Vlasov
- Heat equation

1 domain



9 domains



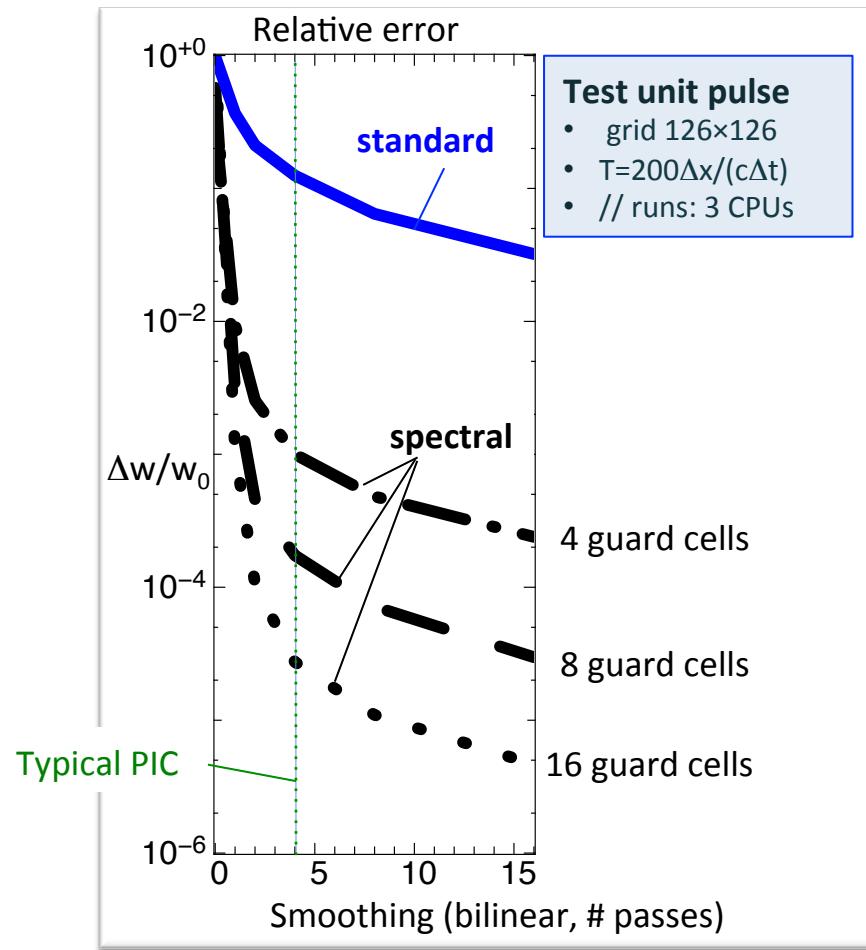
- Diffusion equation
- Vlasov equation
- General relativity
- Schrödinger equation
- any initial value problem(?)

Challenge

-- novel method makes a small approximation

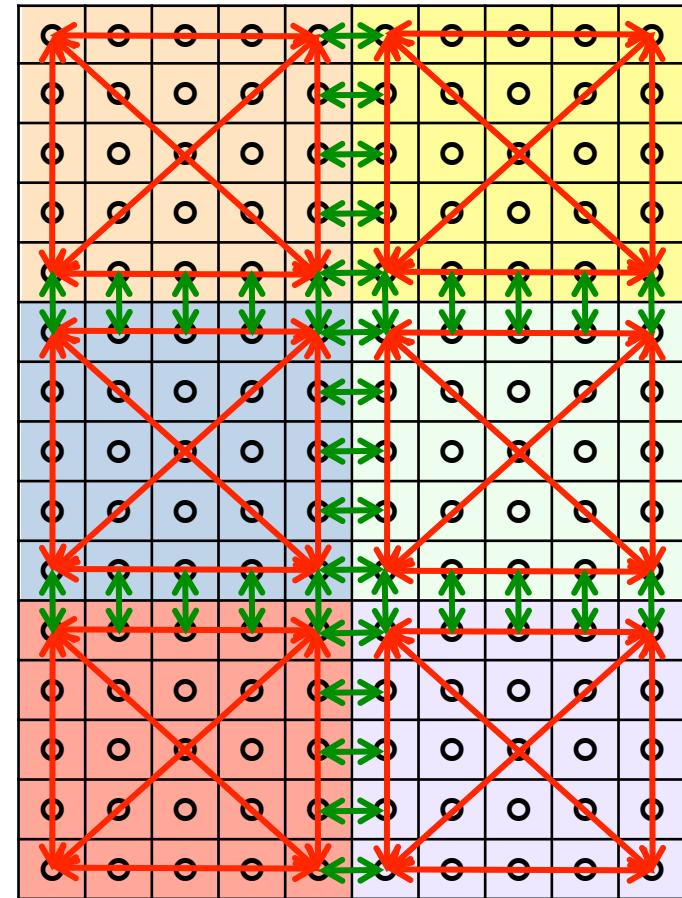
Errors appear lower than standard PIC

e.g., smoothing, guards cells are effective



Mix global with new local exchanges

reduces further impact of approximation



Future directions: error accumulations and mitigations will be studied in detail.



Summary



- **Analytic spectral solver (PSATD) offers higher accuracy, stability & larger Δt**
- **New method uses finite speed of light to allow use of local FFTs**
 - enables scaling of FDTD with accuracy and stability of spectral
- **Prototype implemented in 2-D in Warp**
- **Successfully tested on small unit pulse and laser plasma acceleration runs**
- **May be applicable to other initial value problems**
- **Small approximation could be an issue & further testings are underway**